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On the Calculation of the Exact Number of Zeroes of a Set of Equations

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Abstract — Zusammenfassung

On the Calculation of the Exact Number of Zeroes of a Set of Equations. The number of simple zeroes common to a set of nonlinear equations is calculated exactly and analytically in terms of an integral taken over the boundary of the domain of interest. The integrand consists only of simple algebraic quantities containing the functions involved as well as their derivatives up to second order. The numerical feasibility is shown by some computed examples.

Zur Berechnung der genauen Zahl von Nullstellen eines Gleichungssystems. Die genaue Anzahl der einfachen Nullstellen eines Systems nichtlinearer Gleichungen wird analytisch durch ein Integral über die Berandung des interessierenden Bereichs dargestellt. Der Integrand besteht aus einfachen algebraischen Größen, die die Funktionen samt ihren Ableitungen bis zur zweiten Ordnung enthalten. Die numerische Anwendbarkeit wird mit durchgerechneten Beispielen belegt.

1. Introduction

In many different fields, such as statistics, applied mathematics, physics and engineering, the problem arises of finding the absolute minimum or maximum of a function of one or more parameters. A well-known example is the estimation of unknown parameters by minimizing the difference between experimental data and a theoretical function of the unknown parameters. The mathematical problem of function-minimization has drawn a lot of attention and has evolved to a rather specialized branch of numerical mathematics.

In practice, the determination of the extreme of a function often leads to complicated nonlinear programming problems. It is for instance not uncommon to discover that the function to be optimized has several local extrema. It is in this case a far from trivial problem to obtain the global optimum numerically.

In this contribution we describe a method by which the exact number of stationary points of the function to be optimized can be calculated in the domain of interest. The method requires a relatively small amount of extra computational effort compared with the zero-locating algorithms. However, the extra amount of

computation is justified because the knowledge of the number of stationary points is of great importance for achieving the global optimum. This advantage becomes more conspicuous the larger the number of parameters involved: The function to be optimized cannot be visualized so easily in this case. The method described below originates from the end of the nineteenth century but was forgotten because the analytical computation of the integrals involved is usually prohibitively complicated. Nowadays the required integrations can be carried out numerically by a digital computer. The fundamental concept of the theory of this contribution is the generalization of the concept of the solid angle, given by the Kronecker integral viz. eq. (3) (Kronecker [1]). This integral also occurs in algebraic topology. It is written there in a form independent of a coordinate system on integrating an alternating differential form, Schwartz [2]. The theory of the Kronecker integral is presently known as degree-theory and has many important applications in functional analysis for obtaining e.g. existence theorems, Schwartz [2], Ortega and Rheinboldt [3], Hutson and Pym [4], Sattinger [5].

The Kronecker integral, eq. (3), is not suitable for obtaining the number of zeroes in a domain because its value is equal to the number of zeroes with positive Jacobian minus the number of zeroes with negative Jacobian, i.e. *not conclusive*. It is the forgotten very elegant extension of the theory by Picard [6], viz. the corollary formulated in section 2, which makes the Kronecker integral applicable for the calculation of the number of zeroes.

2. Theory

Let $F(\underline{x})$ be a real function of n real parameters $\underline{x}=(x_1, \dots, x_n)$ which is to be minimized in a certain domain of interest of the \underline{x} -space. We therefore seek the stationary points, defined by:

$$\frac{\partial}{\partial x_j} F(\underline{x}) \equiv f_j(\underline{x}) = 0, \quad j=1, \dots, n \quad (1)$$

in the domain of interest. We consider the problem to find the number of zeroes N common to the set of n eqs. (1).

We will give an intuitive discussion of a theorem and its corollary, derived by Picard [6], which allows the exact calculation of the number of zeroes common to the set of eqs. (1) in the domain of interest.

Theorem:

Let the functions $f_j(\underline{x})$, $j=1, \dots, n$, $\underline{x}=(x_1, \dots, x_n)$ be defined and two times continuously differentiable in a bounded domain D_n of \mathbb{R}_n with boundary S_n .

Suppose that the set of eqs.:

$$f_j(\underline{x}) = 0, \quad j=1, \dots, n \quad (2)$$

only has simple zeroes \underline{x}_l , $l=1, \dots, N$, not located on S_n . Consider the surface integral I_n (Kronecker integral) taken over the surface S_n :

$$I_n = \iint_{S_n} \dots \int \frac{\sum A_i dx_1 \dots dx_{i-1} dx_{i+1} \dots dx_n}{(f_1^2 + f_2^2 + \dots + f_n^2)^{\frac{1}{2}n}}, \quad (3)$$

with

$$A_i = \begin{vmatrix} f_1 & \frac{\partial f_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial x_{i-1}} & \frac{\partial f_1}{\partial x_{i+1}} & \dots & \frac{\partial f_1}{\partial x_n} \\ f_2 & \frac{\partial f_2}{\partial x_1} & \dots & \frac{\partial f_2}{\partial x_{i-1}} & \frac{\partial f_2}{\partial x_{i+1}} & \dots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ f_n & \frac{\partial f_n}{\partial x_1} & \dots & \frac{\partial f_n}{\partial x_{i-1}} & \frac{\partial f_n}{\partial x_{i+1}} & \dots & \frac{\partial f_n}{\partial x_n} \end{vmatrix}, \quad (4)$$

if n is even. A_i equals the determinant (4) multiplied by $(-1)^{i-1}$ if n is odd. I_n is equal to Ω_n times the number of zeroes of the set of eqs. (2) for which the Jacobian $J(\underline{x}_i)$:

$$\frac{\partial(f_1, f_2, \dots, f_n)}{\partial(x_1, x_2, \dots, x_n)}$$

is positive minus the number of zeroes for which the Jacobian is negative. The number Ω_n denotes the surface of a hypersphere with radius unity in \mathbb{R}_n :

$$\Omega_n = \frac{2\pi^{\frac{1}{2}n}}{\Gamma(\frac{1}{2}n)}. \quad (5)$$

Corollary:

Consider a space $\mathbb{R}_{n+1}: x_1, x_2, \dots, x_n, z$. Let $J(\underline{x})$ denote the Jacobian of the set of eqs. (2). Suppose that the zeroes of the set of equations:

$$f_j(\underline{x}) = 0, j = 1, \dots, n; zJ(\underline{x}) = 0; \underline{x} = (x_1, \dots, x_n), \quad (6)$$

contained within an $n+1$ dimensional domain D_{n+1} of \mathbb{R}_{n+1} are simple and not located on the boundary S_{n+1} of D_{n+1} . The total number of zeroes of (6) contained within D_{n+1} is then equal to the integral I_{n+1} (see (3)), taken over S_{n+1} with $f_{n+1}(\underline{x}) \equiv zJ(\underline{x})$.

This number of zeroes is equal to N , viz. the number of zeroes of the set of eqs. (2), if the domain D_{n+1} is the direct product of the domain D_n with an arbitrary interval of the real z -axis containing the point $z=0$.

The proof of this corollary is immediately obtained from the preceding theorem, if we observe that the Jacobian of (6) is equal to $J^2(\underline{x})$, i.e. a positive definite quantity. (The zeroes are supposed to be simple, i.e. $J(x_l) \neq 0, l = 1, \dots, N$). \square

The proof of the theorem can be obtained by observing that:

$$\nabla \cdot \{(f_1^2 + f_2^2 + \dots + f_n^2)^{-\frac{1}{2}n} A\} \equiv \sum_{i=1}^n \frac{\partial}{\partial x_i} \{(f_1^2 + f_2^2 + \dots + f_n^2)^{-\frac{1}{2}n} A\} = 0, \quad (7)$$

where $A = (A_1(\underline{x}), A_2(\underline{x}), \dots, A_n(\underline{x}))$ are defined in eq. (4). The eq. (7) can be immediately verified by a tedious, though elementary, straightforward calculation, or by complete induction. We can therefore, by Gauss' theorem, change the integral into a sum of very small spherical surfaces s_i surrounding the singularities of the integrand, i.e. the roots of eqs. (2):

$$\int_{S_n} (f_1^2 + f_2^2 + \dots + f_n^2)^{-\frac{1}{2}n} A(\underline{x}) \cdot \underline{n} d\sigma - \sum_{l=1}^N \int_{s_l} (f_1^2 + f_2^2 + \dots + f_n^2)^{-\frac{1}{2}n} A(\underline{x}) \cdot \underline{n} d\sigma =$$

$$= \int_{\tau} \nabla \cdot \{(f_1^2 + f_2^2 + \dots + f_n^2)^{-\frac{1}{2}n} A(\underline{x})\} d\tau = 0, \quad (8)$$

where \underline{n} denotes the normal to the surface S_n and $d\sigma$ is a surface element. The domain τ is bounded by S_n and all the surfaces s_l .

Each of the surface integrals over s_l is equal to plus, or minus Ω_n , depending on the sign on the Jacobian at the point \underline{x}_l , as was shown by Picard [7], taking the limit of infinitesimally small spherical surfaces. This leads to the desired result.

It is to be expected that the value of the integral is unchanged when the integration surface is deformed in such a way that no singularities of the integrand are crossed, as will be shown in the following. With the transformation:

$$X_j = f_j(\underline{x}); \quad j = 1, 2, \dots, n, \quad (9)$$

the integral I_n (eq. (3)) reads as:

$$I_n = \int_{S_n} \underline{n} \cdot \nabla V d\sigma, \quad (10)$$

where:

$$V(\underline{X}) = \begin{cases} \log r, & n=2 \\ r^{-n+2}, & n=3, 4, \dots \end{cases}; \quad r^2 = X_1^2 + X_2^2 + \dots + X_n^2. \quad (11)$$

V satisfies the n -dimensional inhomogeneous equation of Laplace:

$$\nabla^2 V = \delta(\underline{X}), \quad \underline{X} = (X_1, X_2, \dots, X_n). \quad (12)$$

The value of (10) is invariant under a transformation of the surface S_n into S'_n provided no singularity of the integrand is crossed during the deformation of the surface, because it denotes the solid angle with respect to the origin in n -dimensional space, Schwartz [2]. See also Kaplan [8] for a discussion in \mathbb{R}_3 . The analytical proof of the invariance property is obtained from Gauss' theorem and eq. (9):

$$\int_{S_n} \underline{n} \cdot \nabla V d\sigma = \int_{S'_n} \underline{n} \cdot \nabla V d\sigma + \int_{\tau} \nabla \cdot \nabla V d\tau, \quad (13)$$

where τ denotes the domain in \mathbb{R}_n bounded by S_n and S'_n , not containing a singularity of the integrand. The last term at the r.h.s of eq. (13) vanishes by virtue of (9), so that eq. (13) proves the desired invariance property. □

The integral (3) was introduced by Kronecker [1] and is in his honour henceforth called: Kronecker integral. A discussion of the Kronecker integral in \mathbb{R}_3 is given by Kaplan [8].

In this contribution we will not consider the case in which the set of eqs. (2) admits multiple zeroes. We will treat this problem in a forthcoming paper, using some interesting ideas put forward by Davidoglou [9] and Tzitzéica [10].

3. Examples

In this section we present some numerical examples of the foregoing theory. The number of simple zeroes in various domains are calculated in the case of equations of one or two variables. All computations were performed on a CDC Cyber 170/760, the programming was done in Fortran.

Example 1: The number of zeroes N of the following equation:

$$f(x) \equiv J_0(x) + J_1(x) = 0, \quad (14)$$

is calculated in the interval (a, b) of the real axis (a and b arbitrarily chosen).

In (14) $J_0()$ and $J_1()$ denote the zero-order and first-order Bessel function, respectively. Precautions should be taken to avoid that $f(a) = 0$ or/and $f(b) = 0$, as will be clarified. The function $f(x)$ is shown in Fig. 1 in the interval $(-10.0, 30.0)$.

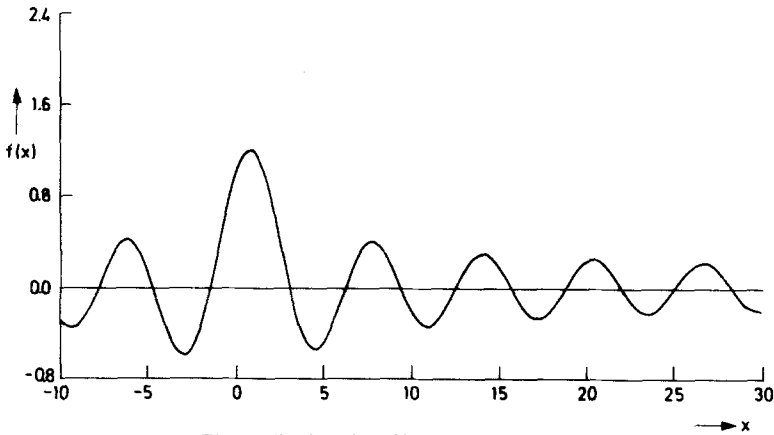


Fig. 1. The function $f(x) = J_0(x) + J_1(x)$

In order to calculate N we apply the recipe of eq. (6) and consider the two equations:

$$\begin{aligned} f(x) &= 0 \\ y f'(x) &= 0, \end{aligned} \quad (15)$$

where $f'(x)$ denotes the derivative of $f(x)$. (Remark that (15) has the same number of zeroes as (14), provided $y \neq 0$.)

We therefore calculate the Kronecker integral (3) of the two eqs. (15), along the sides of the rectangular domain in the xy -plane given by: $a \leq x \leq b$; $-\varepsilon \leq y \leq \varepsilon$ with ε an arbitrary, small positive constant. The number of simple zeroes N of (15) in the rectangle is given by [6]:

$$\begin{aligned} N = & -(\pi)^{-1} \varepsilon \int_a^b \frac{f(x)f''(x) - f'^2(x)}{f^2(x) + (\varepsilon f'(x))^2} dx + (\pi)^{-1} \arctan \left(\frac{\varepsilon f'(b)}{f(b)} \right) \\ & - (\pi)^{-1} \arctan \left(\frac{\varepsilon f'(a)}{f(a)} \right), \end{aligned} \quad (16)$$

a result which is immediately obtained from the corollary on integrating (3) along the rectangle. It has been explicitly shown by Picard [6] that the r. h. s. of eq. (16) is independent of ε , as is to be expected. From (16) we also see why a zero located at a or/and b should be avoided. N is calculated numerically from (16) with the help of an integration routine from the NAG-library. The results of the computations for various values of a and b are given in Table 1. In all cases the first eight decimals of N were equal to zero, ε was set equal to 1.0. The computational time was about .5 seconds for each interval.

Table 1. *The number of zeroes N of $J_0(x) + J_1(x)$ in (a, b)*

a	b	N
-10.0	2.0	3.
-7.0	0.0	2.
-5.0	7.0	4.
5.0	25.0	6.
-10.0	30.0	12.

Example 2: The number of simple zeroes N common to the following set of equations is calculated within a domain D_2 with contour C_2 in the xy -plane:

$$\begin{aligned} f(x, y) &= \sin(2\pi(x - y)) = 0 \\ g(x, y) &= \sin(2\pi(x + y)) = 0 \end{aligned} \quad (17)$$

In order to calculate N , we now apply Picard's method and consider the set of equations:

$$\begin{aligned} f(x, y) &= 0 \\ g(x, y) &= 0 \\ zJ(x, y) &= 0, \end{aligned} \quad (18)$$

where $J(x, y)$ is the Jacobian of (17):

$$J(x, y) = \frac{\partial f}{\partial x} \frac{\partial g}{\partial y} - \frac{\partial f}{\partial y} \frac{\partial g}{\partial x}. \quad (19)$$

We calculate the Kronecker integral (3) of the system (18) over the surface S_3 of the domain D_3 enclosed by the planes $z = \pm\varepsilon$, respectively, and a cylinder whose perpendicular cross-section is bounded by C_2 . From the corollary on integrating (3) along the surface S_3 we immediately obtain [6]:

$$N = (2\pi)^{-1} \int_{C_2} \{Pdx + Qdy\} + \varepsilon(2\pi)^{-1} \iint_{D_2} \frac{R dx dy}{(f^2 + g^2 + \varepsilon^2 J^2)^{3/2}}, \quad (20)$$

where:

$$\begin{aligned}
 P &= \frac{1}{2} \left(f \frac{\partial g}{\partial x} - g \frac{\partial f}{\partial x} \right) \int_{-\varepsilon}^{+\varepsilon} \frac{J}{(f^2 + g^2 + z^2 J^2)^{3/2}} dz = \\
 &= \frac{f \frac{\partial g}{\partial x} - g \frac{\partial f}{\partial x}}{f^2 + g^2} \frac{\varepsilon J}{(f^2 + g^2 + \varepsilon^2 J^2)^{\frac{1}{2}}},
 \end{aligned}
 \tag{21}$$

$$\begin{aligned}
 Q &= \frac{1}{2} \left(f \frac{\partial g}{\partial y} - g \frac{\partial f}{\partial y} \right) \int_{-\varepsilon}^{+\varepsilon} \frac{J}{(f^2 + g^2 + z^2 J^2)^{3/2}} dz = \\
 &= \frac{f \frac{\partial g}{\partial y} - g \frac{\partial f}{\partial y}}{f^2 + g^2} \frac{\varepsilon J}{(f^2 + g^2 + \varepsilon^2 J^2)^{\frac{1}{2}}},
 \end{aligned}
 \tag{22}$$

and R is the following determinant:

$$R = \begin{vmatrix} f \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \\ g \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \\ J \frac{\partial J}{\partial x} & \frac{\partial J}{\partial y} \end{vmatrix}.
 \tag{23}$$

The zeroes common to the equations (17) are shown in Fig. 2 for the domain in the xy -plane: $-1. \leq x \leq +1.;$ $-1. \leq y \leq +1.$

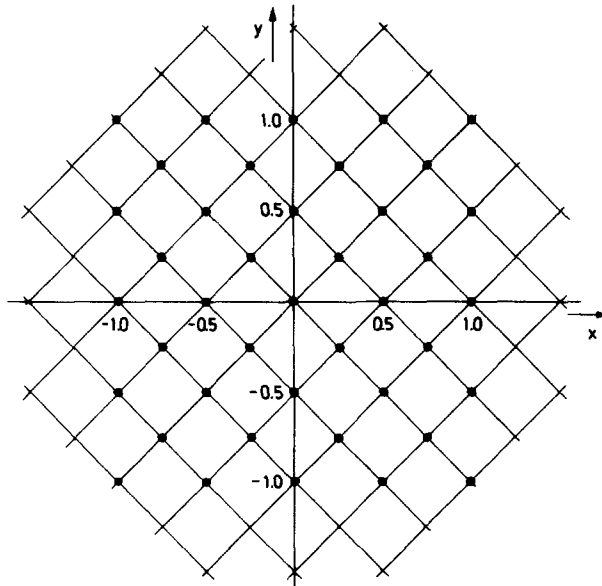


Fig. 2. The curves: $\sin \{2 \pi (x - y)\} = 0$, $\sin \{2 \pi (x + y)\} = 0$

For reasons of computational convenience we took C_2 to be a rectangle. The integration over the surface S_3 now becomes an integration over the sides of a rectangular parallelepiped. The two-dimensional integrations were carried out by an algorithm from the NAG-library. The results of the computation for various rectangles in the xy -plane are summarized in Table 2. In the computations ε was set equal to 10^{-2} , the computational time was about 15 seconds for the calculation of 41 zeroes. Again, the first eight decimals of N were equal to zero.

Table 2. *The number of zeroes N common to: $f(x, y) = \sin(2\pi(x - y)) = 0$, $g(x, y) = \sin(2\pi(x + y)) = 0$ inside the rectangle: $x_a \leq x \leq x_b$; $y_a \leq y \leq y_b$*

x_a	$\leq x \leq$	x_b	y_a	$\leq y \leq$	y_b	N
-1.125		1.125	.125		1.125	18
-.6		1.125	-1.125		1.125	32
.125		1.125	.125		1.125	8
-.8		.8	-.8		.8	25
-1.125		1.125	-1.125		1.125	41

The positions of the sides of the rectangle have been chosen in such a way that zeroes are not located on them. We expect difficulties when a zero is located on the contour C_2 . The denominator in (21) and (22) becomes zero at the pertinent point at the contour for z equal to zero. This leads to convergence problems or a zero division in the numerical evaluation of the integral. A modification of the contour C_2 will remove the singularity from the integrand.

Example 3: Our last example is a function used in [11] for the testing of a numerical procedure for the determination of multiple solutions of nonlinear equations. Branin modified the (well-known) Rosenbrock's function [12] into:

$$h(x, y) = a(y - bx^2 + cx - d)^2 + e(1 - f) \cos x + e. \quad (24)$$

The stationary points of Branin's function (24) are determined by the gradient equations:

$$\begin{aligned} \frac{\partial h}{\partial x} &\equiv f(x, y) = 2a(y - bx^2 + cx - d)(-2bx + c) - e(1 - f) \sin x = 0 \\ \frac{\partial h}{\partial y} &\equiv g(x, y) = 2a(y - bx^2 + cx - d) = 0 \end{aligned} \quad (25)$$

The values of the constants are [11]: $a=1$, $b=5/(4\pi^2)$, $c=5/\pi$, $d=6$, $e=10$ and $f=(8\pi)^{-1}$. The curves $\frac{\partial h}{\partial x}=0$ (drawn line) and $\frac{\partial h}{\partial y}=0$ (dotted line) are shown in Fig. 3 in the region of the xy -plane: $-10.0 \leq x \leq 30.0$; $0.0 \leq y \leq 40.0$.

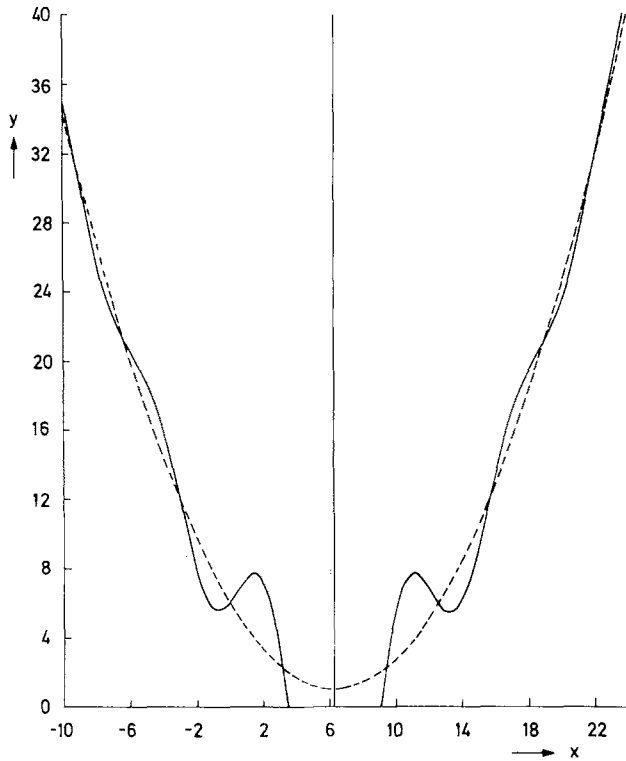


Fig. 3. The curves: $\frac{\partial h}{\partial x}=0$ (drawn line), $\frac{\partial h}{\partial y}=0$ (dotted line)

The computation of the Kronecker integral (3) of the following set of equations:

$$\begin{aligned} f(x, y) &= 0 \\ g(x, y) &= 0 \\ zJ(x, y) &= 0, \end{aligned} \quad (26)$$

results similarly as in the case of example 2, to the number of stationary points of (24) in the domain of interest. The results of the computation for various rectangular domains in the xy -plane are summarized in Table 3. ε was set equal to 5, the computational time was about 28 seconds for a typical parallelepiped.

Table 3. The number of zeroes N common to: $\frac{\partial h}{\partial x}=0$ and $\frac{\partial h}{\partial y}=0$ inside the rectangle: $x_a \leq x \leq x_b$; $y_a \leq y \leq y_b$

x_a	$\leq x \leq$	x_b	y_a	$\leq y \leq$	y_b	N
- 2.0		10.0	.0		40.0	3.9947
-10.0		20.0	.0		30.0	9.0513
-10.0		10.0	.0		25.0	5.9506
-10.0		30.0	.0		25.0	8.9471
-10.0		30.0	.0		40.0	10.9284

4. Discussion

It is a substantial advantage of the method described above that no high accuracy is required in the numerical integrations, because we know in advance that the outcome has to be an integer. As with every numerical integration one faces the danger of accidental convergence for which the usual precautions have to be taken.

All zeroes are located in the part D_n of the hyperplane $z=0$ of D_{n+1} . This makes the integral I_{n+1} defined in the corollary independent of the choice of the range $(-\varepsilon, +\varepsilon)$ of the auxiliary z -axis. One therefore may choose a value of ε which makes the integrand of the Kronecker integral best suitable for numerical integration, i.e. as smooth as possible.

The examples presented are systems of equations with a non-vanishing Jacobian at the common zeroes. The reason for this is that the theory described so far in this contribution is based on this assumption, whereas the extension of the theory to the case of multiple zeroes leads to more complicated integrals (see [9], [10]). It is, however, not uncommon to encounter in practice cases in which multiple zeroes occur [11]. We will therefore in a forthcoming publication extend the theory to this case.

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